

REMARKS/ARGUMENTS

Claim Rejections - 35 USC § 101

The Examiner has not found Applicants' arguments submitted in response to the last and prior Office Actions persuasive and has maintained the 35 U.S.C. § 101 rejection with respect to claims 1 – 3 and claims 10 – 12. While Applicants do appreciate the Examiner's careful analysis and patience, Applicants continue to believe that the claims do define patentable subject matter. Applicants have amended the claims to more specifically define their invention.

Summary of Examiner's Comments and Position:

The Examiner's comments appear to divide themselves into three areas of concern. The first area is summarized as follows:

"Applicant argues that the unspecified, uncharacterized, unsynthesized library of portions of molecules or chemicals represent a statutory category of invention, and that they import functionality to the computer. These arguments are unpersuasive. The molecules themselves do not direct the computer to do anything; they do not impart any order or function on the computer that stores them. No computer actually stores these molecules. These molecules are bits of information stored on the machine. As data, they are indecipherable from any other bits of data. There is a lack of sufficiently identifying information as to what these claims encompass. This is descriptive material that has no computer-related function. Applicant's data does not actually DO anything. The data must be acted upon by something else. Applicant is directed to the new guidelines for computer-related inventions.

The Examiners second area of concern involves whether the invention produces a concrete, tangible and useful result:

For eligibility analysis, physical transformation “is not an invariable requirement, but merely one example of how a mathematical algorithm [or law of nature] may bring about a useful application.” AT&T, 172 F.3d at 1358-59, 50 USPQ2d at 1452... In determining whether the claim is for a “practical application,” the focus is not on whether the steps taken to achieve a particular result are useful, tangible and concrete, but rather that the final result achieved by the claimed invention is “useful, tangible and concrete.” (1) “USEFUL RESULT” For an invention to be “useful” it must satisfy the utility requirement of section 101. The USPTO’s official interpretation of the utility requirement provides that the utility of an invention has to be (i) specific, (ii) substantial and (iii) credible. MPEP § 2107 and Fisher, 421 F.3d at ___, 76 USPQ2d at 1230 (citing the Utility Guidelines with approval for interpretation of “specific” and “substantial”). (2) “TANGIBLE RESULT” The tangible requirement does not necessarily mean that a claim must either be tied to a particular machine or apparatus or must operate to change articles or materials to a different state or thing. However, the tangible requirement does require that the claim must recite more than a § 101 judicial exception, in that the process claim must set forth a practical application of that § 101 judicial exception to produce a real-world result. Benson, 409 U.S. at 7 1-72, 175 USPQ at 676-77 (invention ineligible because had “no substantial practical application.”). “[A]n application of a law of nature or mathematical formula to a ... process may well be deserving of patent protection.” Diehr, 450 U.S. at 187, 209 USPQ at 8 (emphasis added); see also Coming, 56 U.S. (15 How.) at 268, 14 L.Ed. 683 (“It is for the discovery or invention of some practical method or means of producing a beneficial result or effect, that a patent is granted.. .”). In other words, the opposite meaning of “tangible” is “abstract.” (3) “CONCRETE RESULT” Another consideration is whether the invention produces a “concrete” result. Usually, this question arises when a result cannot be assured. In other words, the process must have a result that can be substantially repeatable or the process must substantially produce the same result again. In re Swartz, 232 F.3d 862, 864, 56 USPQ2d 1703, 1704 (Fed. Cir. 2000) (where asserted result produced by the claimed invention is “irreproducible” claim should be rejected

under section 101). The opposite of "concrete" is unrepeatable or unpredictable.

The third area of concern for the Examiner involves whether the virtual library is functional or non-functional descriptive material:

Descriptive material can be characterized as either "functional descriptive material" or "non-functional descriptive material." In this context, "functional descriptive material" consists of data structures and computer programs which impart functionality when employed as a computer component. (The definition of "data structure" is a "physical or logical relationship among data elements, designed to support specific data manipulation functions." The New IEEE Standard Dictionary of Electrical and Electronics Terms 308 (5th ed. 1993).) "Nonfunctional descriptive material" includes but is not limited to music, literary works and a compilation or mere arrangement of data.

Both types of "descriptive material" are nonstatutory when claimed as descriptive material per *Se. Warmerdam*, 33 F.3d at 1360, 31 USPQ2d at 1759. When functional descriptive material is recorded on some computer-readable medium it becomes structurally and functionally interrelated to the medium and will be statutory in most cases since use of technology permits the function of the descriptive material to be realized. When nonfunctional descriptive material is recorded on some computer-readable medium, in a computer or on an electromagnetic carrier signal, it is not statutory since no requisite functionality is present to satisfy the practical application requirement. Merely claiming nonfunctional descriptive material, i.e., abstract ideas, stored in a computer-readable medium, in a computer, on an electromagnetic carrier signal does not make it statutory. See *Diehr*, 450 U.S. at 185-86, 209 USPQ at 8 (noting that the claims for an algorithm in *Benson* were unpatentable as abstract ideas because "[t]he sole practical application of the algorithm was in connection with the programming of a general purpose computer."). Such a result would exalt form over substance. In *re Sarkar*, 588 F.2d 1330, 1333, 200 USPQ 132, 137 (CCPA 1978)...

(b) Nonfunctional Descriptive Material

Nonfunctional descriptive material that does not constitute a statutory process, machine, manufacture or composition of matter and should be rejected under 35 U.S.C. § 101. Certain types of descriptive material, such as music, literature, art, photographs and mere arrangements or compilations of facts or data, without

any functional interrelationship is not a process, machine, manufacture or composition of matter. Nonfunctional descriptive material may be claimed in combination with other functional descriptive multimedia material on a computer-readable medium to provide the necessary functional and structural interrelationship to satisfy the requirements of 35 U.S.C. § 101.

Applicants will address the areas of concern raised by the Examiner. First, Applicants note that the Examiner's first and third points are intimately tied together in that they concern what information is stored in the computer and how that information may be utilized. Specifically, Applicants submits that it is the structure of the virtual library that meets the requirement for functional descriptive material, specifically, a data structure that has a "...logical relationship among the elements, designed to support specific data manipulation functions." The virtual library does not consist of just molecules as would be found in any chemical text or reference book. Such a listing would be of little value in three dimensional shape searching.

Rather, the virtual library is constructed by taking molecular parts, side chains and cores, and applying one or more molecular structural descriptors (metrics) to characterized the parts in a way that reflects the three dimensional shape of those molecular parts. Importantly, not only are the parts characterized in a way that reflects their three dimensional shape in a biologically relevant manner, but the characterization is such that the individual shape characterization of each part can be combined with shape characterizations of other parts to yield an accurate characterization of the shape of a molecule assembled from those parts. It is

these characterized descriptions which are stored in the virtual library. The position of the open valence or attachment bond of each part is also retained in the virtual library as well as the chemical reactions in which that part could participate. Because of this interrelated data, the shape analysis of possible combinatorially assembled product molecules will be chemically meaningful.

There is, thus, a logical relationship among the elements of the virtual library designed to support a specific data manipulation function, namely the characterization of the three dimensional shape of a product molecule which could be combinatorially synthesized from the characterized parts without the necessity of actually forming the molecule in the computer. A further data manipulation function is supported by the virtual library. Specifically, the virtual library enables the characterization of query molecule fragments with the same metric descriptors used in the creation of the virtual library and comparison of the characterized query fragments to the characterized parts in the virtual library. Virtual library parts similar in three dimensional shape to parts of the query molecule can be identified and the shape of a molecule which could be assembled from different parts in the virtual library can be compared to the three dimensional shape of the query molecule without the necessity of constructing in the computer a representation of the combined molecular parts. Applicant respectfully submits that the virtual library consists of functional descriptive material.

It should be noted that the virtual library is created and stored in the readable memory of a computer. (See specification, Section 1, "Computational Chemistry Environment.")

Applicant has amended the preambles to the claims to recite that the virtual library is stored on computer readable medium. Applicant respectfully submits that such functional descriptive material as the virtual library when stored on a computer readable medium meets all requirements for statutory subject matter.

Addressing next the Examiner's comment that the invention does not produce a concrete, tangible result, and useful result. Applicants will respond to each of the three criteria. As noted, USEFULL in the context of the USPTO's interpretation of the utility requirement means that the utility of an invention has to be (i) specific, (ii) substantial and (iii) credible. As noted in Applicants' earlier Responses, the virtual library permits questions to be asked and answered that could not previously been considered. Applicants pointed out in their prior Response that modern biochemistry recognizes the importance of molecular shape as a principal feature of biochemical interactions. The virtual library of this invention was designed to permit three dimensional shape searching, a very specific, substantial, and credible improvement over the prior art. Starting with a known molecule having some desired activity, the question can be posed: what other molecules have the same three dimensional shape as the known molecule? As noted above, during the search process utilizing the virtual library in computer readable memory, the three dimensional shapes of potential molecules, which can be calculated from the characterized molecular parts in the virtual library through a combination of the individual descriptor values, can be compared to the shape of the query molecule without the necessity of generating the product structures. Applicants submit that the "Useful" criteria are fully met.

TANGIBLE means that the claim must set forth an implementation to produce a real-world result. The identification of molecules which, when combinatorially (according to known reactions in which they participate) assembled from known reagents (the basis for the parts in the virtual library), will have the same three dimensional shape and likely biological activity of a query molecule (typically a lead compound) is a tangible result. It is not abstract. It is tied to a specific characterized molecular characteristic, namely three dimensional shape. Applicants respectfully submit that the "Tangible" criteria is fully met.

"CONCRETE" requires that there be predictability to the invention. That is certainly the case here. A virtual library which is constructed using the same molecular parts, characterizing metrics, and combinatorial reactions will be identical to and yield the same results as another virtual library formed from the same constituents. Further, a search of each such constructed library will yield the same information about the three dimensional shaped molecules which are similar to the same query molecule. Applicants respectfully submit that the "Concrete" criteria is fully met.

Finally the Examiner has continued the rejection under 35 U.S.C. § 102(e) as being anticipated by Agrafiotis or Horlbeck. In view of Applicants' arguments presented above with respect to the fact that the virtual library is functional descriptive material (data structures), Applicants request the Examiner to review Applicants' previous arguments with respect to distinguishing Agrafiotis and Horlbeck. In particular, neither Agrafiotis nor Horlbeck characterize molecular parts with metrics which have been shown to be biologically relevant. As

noted above, the virtual library of this invention is not comprised of molecules or simply of molecular parts. The data structure of the virtual library contains three dimensional metric characterizations of the molecular parts which permits three dimensional shape searching. Neither Agrafiotis nor Horlbeck enable searching in 3D for molecules of similar shape, especially without the necessity of assembling the molecule. Applicant respectfully submits that neither Agrafiotis or Horlbeck anticipate Applicants' invention.

In addition to the arguments presented here, Applicants incorporate herein Applicants' comments and descriptions of Applicants' invention set forth in Applicants' prior Responses. With the amendment of the claims and the arguments set forth above, Applicants submit that they have adequately addressed all grounds for rejection raised by the Examiner and respectfully request that a timely Notice of Allowance be issued in this case.

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Respectfully submitted,



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